

A k- ω -MULTIVARIATE BETA PDF FOR SUPERSONIC COMBUSTION

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Introduction

In an attempt to study the interaction between combustion and turbulence in supersonic flows, an assumed PDF has been employed^{1,2}. This makes it possible to calculate the time average of the chemical source terms that appear in the species conservation equations as

$$\bar{\dot{w}_s} = \int P(T, Y_1, \dots, Y_n) \dot{w}_s dT dY_1 \dots dY_n \quad (1)$$

where \dot{w}_s is the production rate of species s , P is the probability density function, T is the temperature and Y_k is the mass fraction of species k . The probability density function is assumed to have the form

$$P(T, Y_1, \dots, Y_n) = F_1(T) F_2(Y_1, \dots, Y_n)$$

where F_1 is a Gaussian distribution and F_2 is the multivariate PDF developed by Girimaji³, i.e.,

$$F_2(Y_1 \dots Y_n) = \frac{1}{c} \delta(1-s) \prod_{k=1}^n Y_k^{\beta_k-1}$$

where

$$s = \sum Y_k, \quad c = \prod_{k=1}^n \Gamma(\beta_k) / \Gamma(\sum \beta_k)$$

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δ is the Dirac delta function, and n is the number of species present. The quantities β_k appearing in the PDF can be determined in terms of the mean mass fractions and the sum of their variances, i.e.,

$$\beta_k = \bar{Y}_n \left(\frac{1-S}{Q} - 1 \right) \quad (5)$$

where

$$S = \sum (\bar{Y}_k)^2, \quad Q = \sum \bar{Y}_k'^2 \quad (6)$$

In order to determine the averages indicated in equation (1), two transport equations, one for the temperature (enthalpy) variance and one for Q , are required. Model equations are formulated for such quantities and they can be written as

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{h}'^2) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{h}'^2) = \frac{\partial}{\partial x_j} \left[\left(\frac{\mu}{\bar{\rho} Pr} + \frac{\mu_t}{\bar{\rho} Pr_t} \right) \frac{\partial}{\partial x_j} (\bar{\rho} \bar{h}'^2) \right] + 2C_1 \frac{\mu_t}{Pr} \left(\frac{\partial \bar{h}}{\partial x_j} \right)^2 - \frac{\bar{\rho} \bar{h}'^2}{\tau} \quad (7)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Q}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{Q}) = \frac{\partial}{\partial x_j} \left[\bar{\rho} (D + D_t) \frac{\partial \bar{Q}}{\partial x_j} \right] + 2 \bar{\rho} D_t \left(\frac{\partial \bar{Y}_k}{\partial x_j} \right)^2 + 2 \sum \bar{\omega}_k \bar{Y}_k'' - C_Q \frac{\bar{\rho} \bar{Q}}{\tau} \quad (8)$$

In the above equation D is the diffusion coefficient, μ is the viscosity, C_1 and C_Q are model constants and τ is the turbulent time scale.

As is seen from equations (7) and (8), the turbulent time scale controls the evolution of both $(\bar{h}')^2$ and \bar{Q} . An algebraic model similar to that used by Eklund et al.⁴ was used in Reference 2 in an attempt to predict the recent measurements of Cheng et al.⁵ Predictions were satisfactory before ignition but were less satisfactory after ignition. One of the reasons for this behavior is the inadequacy of the algebraic turbulence model employed. Because of this, the objective of this work is to develop a k - ω model to remedy the situation.

Results and Discussion

A full kinetic model based on the work of Jachimowski⁶ is employed. It consists of eighteen reactions (Table 1) and allows for the presence of H_2 , O_2 , H , O , OH , H_2O , HO_2 , H_2O_2 and treats N_2 as an inert. A schematic of the experimental setup is shown in Figure 1, and Table 2 gives a summary of the burner exit conditions. Measurements were taken at axial locations of 0.85, 10.8, 21.5, 32.3, 43.1, 64.7, and 86.1 inner diameters downstream of the burner.

It became evident that traditional model constants in the $k-\omega$ model were not appropriate for modeling the experiment under consideration. Because of this, we decided to develop, as a first step, a one-equation turbulence model based on the energy equation and then use it to develop the $k-\omega$ model. This first step is now complete.

Figures 2-4 show comparisons of mean temperature, mean H_2O , and rms H_2O distributions. As is seen from the figures, there is a need to implement the full $k-\omega$ model.

The paper will implement the complete turbulence model and will present detailed comparisons with the measurements of Ref. 5.

Acknowledgement

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Tables

Table 1. Chemistry Model

Reaction Number	Reaction	A	b	E_a
1	$H_2 + O_2 \rightarrow OH + OH$.170E + 14	0.00	24157.0
2	$H + O_2 \rightarrow OH + O$.120E + 18	-0.91	8310.5
3	$OH + H_2 \rightarrow H_2O + H$.220E + 14	0.00	2591.8
4	$O + H_2 \rightarrow OH + H$.506E + 05	2.67	3165.6
5	$OH + OH \rightarrow H_2O + O$.630E + 13	0.00	548.6
6	$HO_2 + H \rightarrow H_2 + O_2$.130E + 14	0.00	0.0
7	$HO_2 + H \rightarrow OH + OH$.150E + 15	0.00	503.3
8	$HO_2 + O \rightarrow O_2 + OH$.200E + 14	0.00	0.0
9	$HO_2 + OH \rightarrow H_2O + O_2$.200E + 14	0.00	0.0
10	$HO_2 + H_2 \rightarrow H_2O_2 + H$.301E + 12	0.00	9411.2
11	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$.200E + 13	0.00	0.0
12	$H + H_2O_2 \rightarrow H_2O + OH$.100E + 14	0.00	1801.7
13	$O + H_2O_2 \rightarrow HO_2 + OH$.280E + 14	0.00	3220.9
14	$OH + H_2O_2 \rightarrow H_2O + HO_2$.700E + 13	0.00	722.2
15	$H + OH + M \rightarrow H_2O + M$.221E + 23	-2.00	0.0
16	$H + H + M \rightarrow H_2 + M$.730E + 18	-1.00	0.0
17	$H + O_2 + M \rightarrow HO_2 + M$.230E + 19	-1.00	0.0
18	$H_2O_2 + M \rightarrow OH + OH + M$.121E + 18	0.00	22898.8

Units of A are a multiple of $cm^3 \cdot mole^{-1} \cdot s^{-1}$

Table 2. Exit Conditions

Exit Conditions	Hydrogen Jet	Outer Jet	Ambient Air
Mach Number	1.0	2.0	0.
Temperature, K	545	1250	300
Velocity, m/s	1780	1417	0.
Pressure, MPa	.112	.107	.101
Mass Fraction			
Y_{H_2}	1.	0.	0.
Y_{O_2}	0.	.245	.233
Y_{N_2}	0.	.58	.757
Y_{H_2O}	0.	.175	0.01

Figures

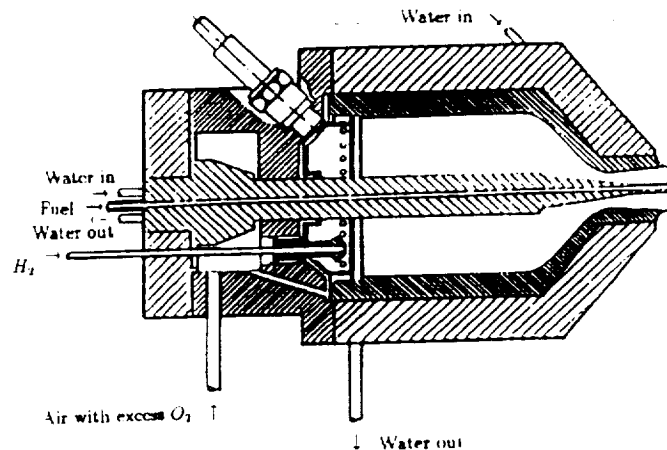


Figure 1: Schematic of test apparatus

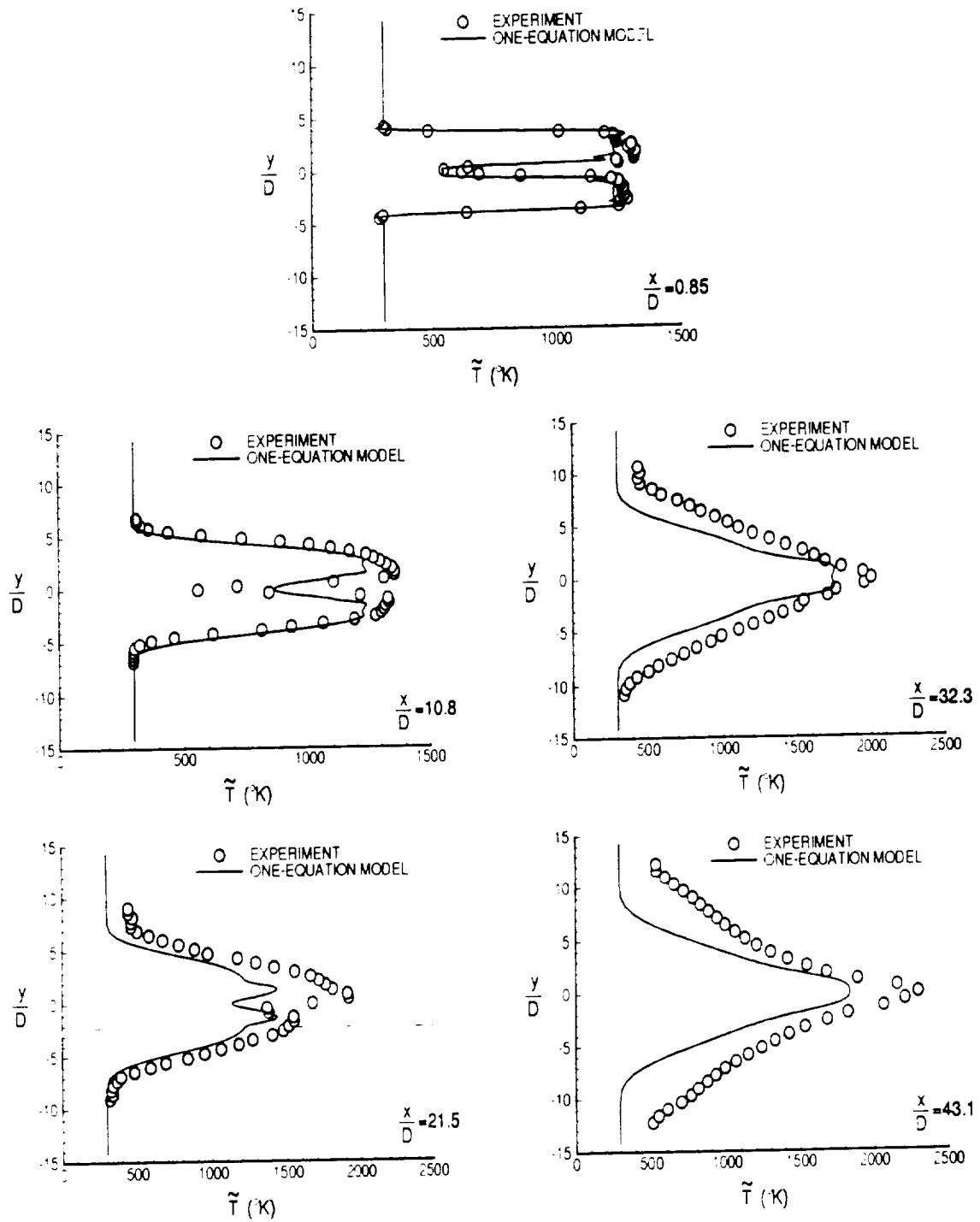


Figure 2: Mean Temperature Comparison With Experiment

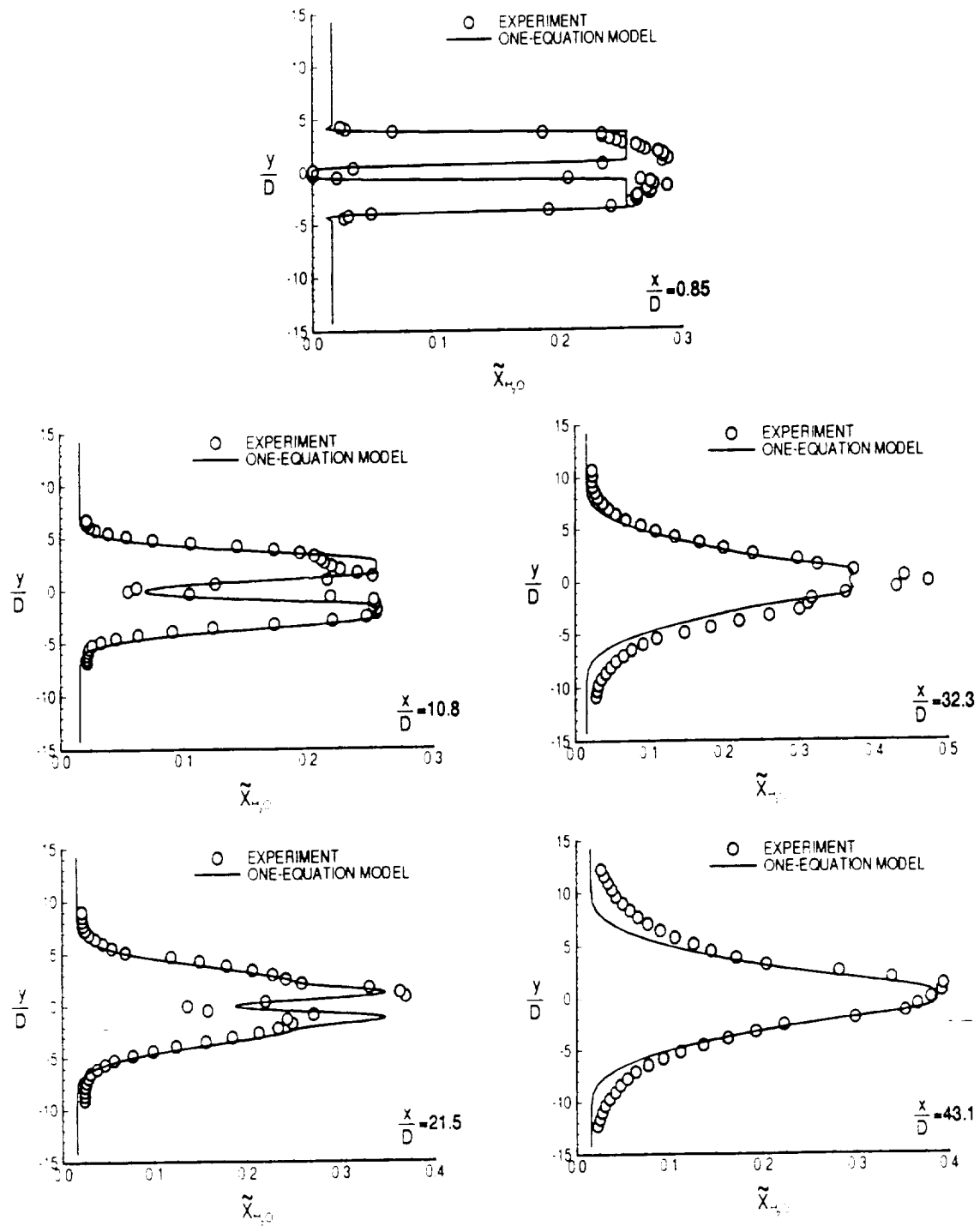


Figure 3: Mean H_2O Mole Fraction Comparison With Experiment

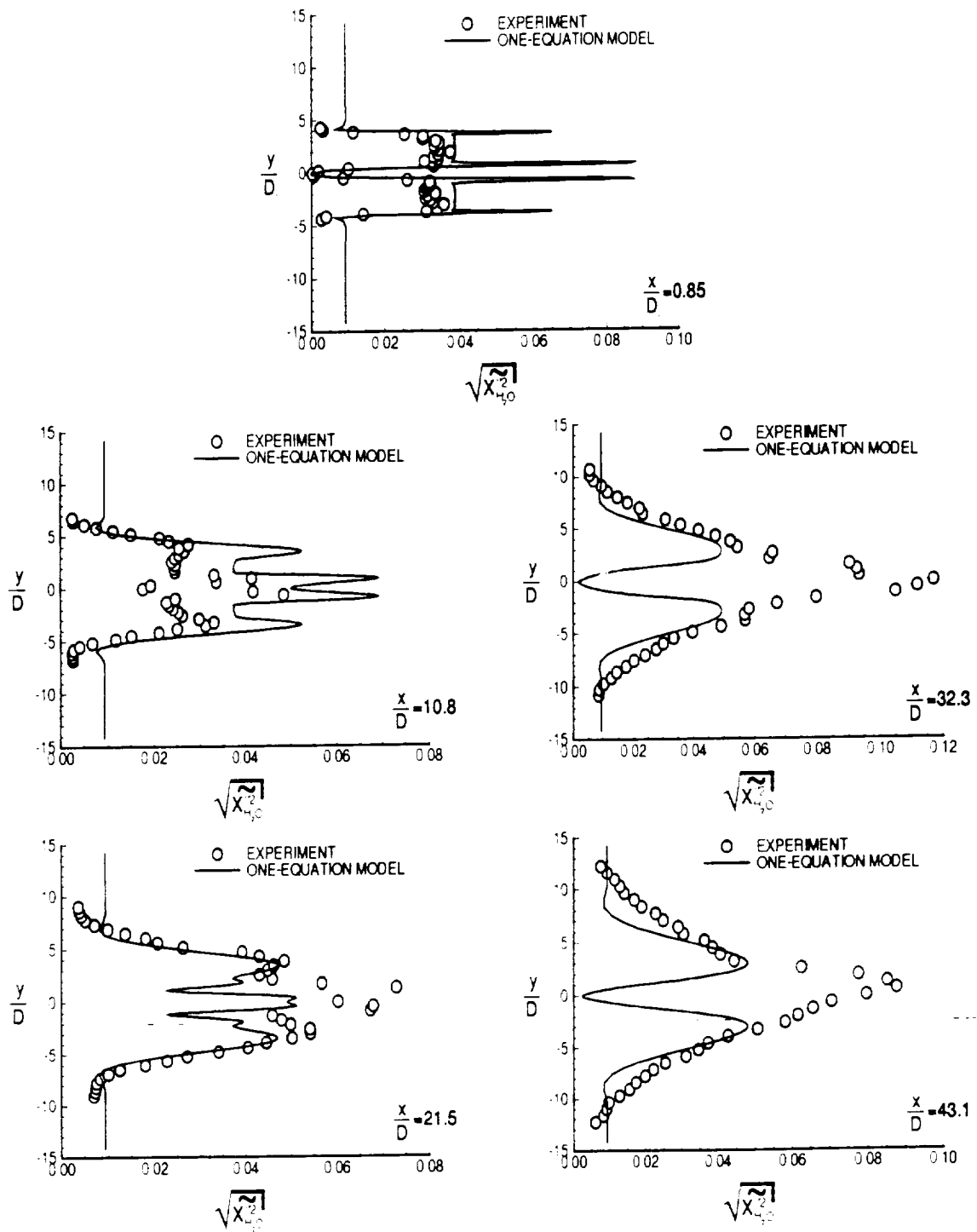


Figure 4: RMS H_2O Mole Fraction Comparison With Experiment